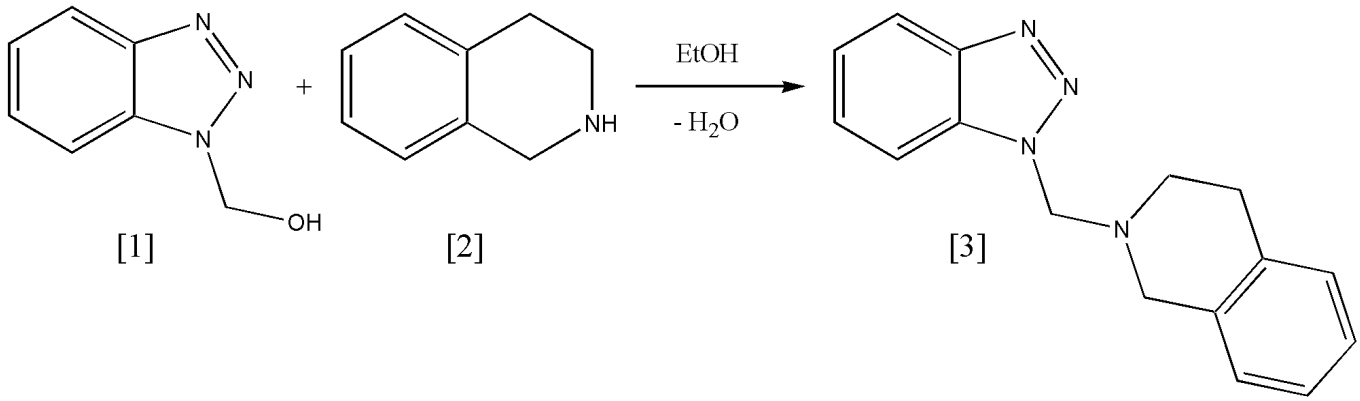
Molecules **1999**, *4*, M91

N-Benzotriazol-1-yl-methyl-1,2,3,4-tetrahydroisoquinoline

Cornelia Locher*, Sara Baldey and Naseem Peerzada*

Faculty of Science, Northern Territory University, Darwin, N.T. 0909, Australia - ph: 0061-8-8946 6850, fax: 0061-8-8946 6847, e-mails (Cornelia Locher) clocher@banda.ntu.edu.au, (Sara Baldey) sbaldey@banda.ntu.edu.au, (Naseem Peerzada) peerzadan@banks.ntu.edu.au

Received: 16 October 1998 / Published: 22 February 1999



[1] [2] [3]

Benzotriazole-mediated heteroalkylations have been explored for many synthetic pathways. The principle of an aminoalkylation (or Mannich reaction) with primary or secondary amines was applied to the reaction of 1-hydroxymethylbenzotriazole [1] with 1,2,3,4-tetrahydroisoquinoline [2] which yielded very high quantities of crystalline *N*-benzotriazol-1-ylmethyl-1,2,3,4-tetrahydroisoquinoline [3].

1,2,3,4-Tetrahydroisoquinoline (19.9mmol, 2.64g) was added to 1-hydroxymethylbenzotriazole (2.96g, 19.9mmol) with stirring. Ethanol (5mL) was added and the mixture heated. The reaction was very fast and initial crystallisation of the product started already after a few seconds. More ethanol (15mL) was added and the solution refluxed with stirring for 30min. The mixture was kept at -5 ° C over night, the final product (5.14g, 98%) was collected under reduced pressure and washed with cold ethanol. It was recrystallised from ethanol and yielded *N*-benzotriazol-1-ylmethyl-1,2,3,4-tetrahydroisoquinoline [3] as white needles.

M.p. 155-157 °C (EtOH, uncorrected).

UV l_{max}(nm; EtOH) / e ($dm^3mol^{-1}cm^{-1}$) 206 / 27060, 253 / 6970 and 273 / 5808.

IR n_{max}(cm^{-1}; Nujol) 1260, 1210, 1150, 1090, 1050, 955, 940, 740.

^{1}H-NMR d_H (200 MHz; $CDCl_3$; Me_4Si) 8.08 (1H, d, *J* 4), 7.68 (1H, d, *J* 4), 7.52 (1H, t, *J* 7), 7.38 (1H, t, *J* 7), 7.10-6.90 (4H, m), 5.64 (2H,s, NCH_2N), 3.86 (2H, s, $ArCH_2N$), 2.96-2.91 (4H, m, $ArCH_2CH_2N$).

^{13}C-NMR d_C (50 MHz; $CDCl_3$) 29.0 ($ArCH_2CH_2N$), 48.4 ($ArCH_2N$), 52.3 ($ArCH_2CH_2N$), 69.1 (NCH_2N), 110.1, 118.4, 120.1, 124.1, 125.9, 126.4, 126.6, 127.7, 128.9, 133.6, 133.7, 134.0, 146.1.
Analysis Found ($C_{16}H_{16}N_4$, 264.33, Calc.) C 72.6 (72.7), H 6.2 (6.1), N 21.2 (21.2).

Acknowledgments: One of the authors (C.L.) would like to thank the Northern Territory University for the receipt of a University Postgraduate Research Scholarship.

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Sample Availability: Available from the authors (C.L. or N.P.) and from MDPI. MDPI Reg. No. 15927.